

Energy nonequpartition in a sheared granular mixture

Vicente Garzó

*Departamento de Física, Universidad de Extremadura, E-06071
Badajoz, Spain*

José María Montanero

*Departamento de Electrónica e Ingeniería Electromecánica,
Universidad de Extremadura, E-06071*

Badajoz, Spain

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Abstract

The kinetic granular temperatures of a binary granular mixture in simple shear flow are determined from the Boltzmann kinetic theory by using a Sonine polynomial expansion. The results show that the temperature ratio is clearly different from unity (as may be expected since the system is out of equilibrium) and strongly depends on the restitution coefficients as well as on the parameters of the mixture. The approximate analytical calculations are compared with those obtained from Monte Carlo simulations of the Boltzmann equation showing an excellent agreement over the range of parameters investigated. Finally, the influence of the temperature differences on the rheological properties is also discussed.

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Although experimental and theoretical studies on granular media have been mainly focused on assemblies of identical particles, there appears to be a recent growing interest among both theorists and experimentalists in the more complicated case of polydisperse systems. In this case, several kinetic theory studies in the freely cooling [1] and thermostatted steady [2] states have shown that the kinetic temperatures of each species are different. This violation of energy equipartition has been subsequently confirmed in experiments of vibrated granular mixtures [3]. When the system is sheared, a similar result has been recently found by Clelland and Hrenya [4] from molecular dynamics (MD) simulations of a binary-sized mixture of inelastic, smooth hard disks engaged in rapid shear flow. Their results were compared with previous kinetic theory calculations [5] based on the assumption of equipartition of granular energy. As Clelland and Hrenya conclude [4], although this equipartition-of-energy assumption does not appear to have a negative impact on the ability of those earliest theories to predict the stress tensor in simple shear flow, a *multi-temperature* theory must be more appropriate. In the context of kinetic theory, the only primary attempts to include temperature differences in dense granular mixtures were put forward by Jenkins and Mancini [6] and more recently by Huilin *et al.* [7]. However, both works are phenomenological with no attempt to solve the kinetic equation. Instead, they assume that the velocity distribution functions are local Maxwellians. This can be reasonable to estimate the dense gas collisional transfer contributions to the fluxes, but not to compute their kinetic contributions. On the other hand, both theories are applicable to a general flow field.

The goal of this brief report is to explicitly get the dependence of the temperature ratio $\gamma \equiv T_1/T_2$ on particle properties as well as on compositional parameters of a granular binary mixture subjected to the simple shear flow. The calculation of γ allows one to assess the magnitude of the equipartition violation and its dependence on the parameters of the system. On the other hand, due to the complexity of the general problem, here we will restrict ourselves to the low-density regime in which case the velocity distribution functions f_i for the two species verify a set of two coupled nonlinear Boltzmann equations. This set of equations is first analytically solved by using a first-Sonine polynomial approximation. Then, to check the reliability of our theoretical results, the direct simulation Monte Carlo method [8] is also employed to numerically solve the Boltzmann equation in the shear flow state. As will be shown later, our theory presents a much better agreement with simulations than the one given by Jenkins and Mancini [6].

Let us consider a granular binary mixture composed by smooth inelastic disks or spheres of masses m_1 and m_2 and diameters σ_1 and σ_2 . Collisions between particles are inelastic and characterized by three constant (independent) restitution coefficients α_{11} , α_{22} , and $\alpha_{12} = \alpha_{21}$, where $\alpha_{ij} \leq 1$ refers to the restitution coefficient for collisions between particles of species i and j . The mixture is under simple shear flow, namely, a macroscopic state with a constant linear velocity profile $\mathbf{U} = \mathbf{a} \cdot \mathbf{r}$, where $a_{k\ell} = a\delta_{kx}\delta_{\ell y}$, a being the constant shear rate. In addition, the partial densities n_i and the (global) granular temperature T are uniform. The time evolution of the temperature arises from the balance of two competing effects: viscous heating and collisional cooling. When both mechanisms cancel each other, the system reaches a steady state and the temperature achieves a constant value. This steady state is what we want to analyze here. From a microscopic point of view, the simple shear flow problem becomes spatially uniform in the local Lagrangian frame moving with the flow velocity \mathbf{U} . In this frame, $f_i(\mathbf{r}, \mathbf{v}) \rightarrow f_i(\mathbf{V})$, where $\mathbf{V} = \mathbf{v} - \mathbf{U}$ is the peculiar velocity. Under these

conditions, the set of Boltzmann kinetic equations read

$$-aV_y \frac{\partial}{\partial V_x} f_i(\mathbf{V}) = \sum_j J_{ij}[\mathbf{V}|f_i, f_j], \quad (1)$$

where the Boltzmann collision operator $J_{ij}[\mathbf{V}|f_i, f_j]$ describing the scattering of pairs of particles is

$$J_{ij}[\mathbf{V}_1|f_i, f_j] = \sigma_{ij}^{d-1} \int d\mathbf{V}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \left[\alpha_{ij}^{-2} f_i(\mathbf{V}'_1) f_j(\mathbf{V}'_2) - f_i(\mathbf{V}_1) f_j(\mathbf{V}_2) \right]. \quad (2)$$

Here, d is the dimensionality of the system, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, $\hat{\boldsymbol{\sigma}}$ is a unit vector along their line of centers, Θ is the Heaviside step function and $\mathbf{g}_{12} = \mathbf{V}_1 - \mathbf{V}_2$. In addition, the primes on the velocities denote the initial values $\{\mathbf{V}'_1, \mathbf{V}'_2\}$ that lead to $\{\mathbf{V}_1, \mathbf{V}_2\}$ following a binary collision: $\mathbf{V}'_1 = \mathbf{V}_1 - \mu_{ji} (1 + \alpha_{ij}^{-1}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \hat{\boldsymbol{\sigma}}$ and $\mathbf{V}'_2 = \mathbf{V}_2 + \mu_{ij} (1 + \alpha_{ij}^{-1}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \hat{\boldsymbol{\sigma}}$. Here, $\mu_{ij} = m_i / (m_i + m_j)$.

Our study is focused on the evaluation of the partial temperatures T_i , which measure the mean kinetic energy of each species. In terms of f_i , they are defined as

$$\frac{d}{2} n_i T_i = \int d\mathbf{V} \frac{1}{2} m_i V^2 f_i. \quad (3)$$

The temperature of the mixture is $T = x_1 T_1 + x_2 T_2$, where $x_i = n_i / (n_1 + n_2)$ is the mole fraction of species i . The balance equation of the granular temperature for species i can be obtained by multiplying the Boltzmann equations (1) by $m_i V^2$ and integrating over \mathbf{V} . The result is

$$aP_{i,xy} + \frac{d}{2} \zeta_i p_i = 0, \quad (4)$$

where $p_i = n_i T_i$,

$$\mathbf{P}_i = m_i \int d\mathbf{V} \mathbf{V} \mathbf{V} f_i(\mathbf{V}), \quad (5)$$

is the partial pressure tensor of the species i and $\zeta_i = \sum_j \zeta_{ij}$ is the cooling rate for the partial temperature T_i , with

$$\zeta_{ij} = -\frac{1}{dn_i T_i} \int d\mathbf{V} m_i V^2 J_{ij}[\mathbf{V}|f_i, f_j]. \quad (6)$$

According to Eq. (4), in the steady state the temperature ratio $\gamma \equiv T_1/T_2$ is given by the relation

$$\gamma = \frac{x_2 \zeta_2 P_{1,xy}}{x_1 \zeta_1 P_{2,xy}}. \quad (7)$$

Thus, to get γ one needs to determine the cooling rates ζ_i and the xy element of the partial pressure tensors \mathbf{P}_i . An equation for the elements of \mathbf{P}_i follows immediately from the definition (5) and the Boltzmann equation (1):

$$a_{km}P_{i,m\ell} + a_{\ell m}P_{i,mk} = \sum_j A_{ij,k\ell}, \quad (8)$$

where we have introduced the collisional moments \mathbf{A}_{ij} as

$$\mathbf{A}_{ij} = m_i \int d\mathbf{V} \mathbf{V} \mathbf{V} \mathbf{V} J_{ij}[\mathbf{V}|f_i, f_j]. \quad (9)$$

The determination of \mathbf{P}_i is a closed problem provided the moments \mathbf{A}_{ij} are explicitly known. This requires the knowledge of the velocity distribution functions f_i , which is quite an intricate problem, even in the elastic case. A useful way to estimate ζ_i and \mathbf{A}_{ij} is to expand f_i in Sonine polynomials. This approach is similar to the usual moment method for solving kinetic equations in the elastic case where the leading order truncation is known to be a good approximation. In the case of shear flow, we take the leading Sonine approximation, $f_i(\mathbf{V}) \rightarrow f_{i,M}(\mathbf{V}) [1 + \mathbf{C}_i : \mathbf{D}_i(\mathbf{V})/2T_i]$, where $\mathbf{C}_i = (\mathbf{P}_i/p_i) - \mathbb{1}$ and $\mathbf{D}_i(\mathbf{V}) = m_i [\mathbf{V}\mathbf{V} - (V^2/d)\mathbb{1}]$. Here, $\mathbb{1}$ is the $d \times d$ unit tensor and $f_{i,M}$ is a Maxwellian distribution at the temperature of the species i , i.e.,

$$f_{i,M}(\mathbf{V}) = n_i \left(\frac{m_i}{2\pi T_i} \right)^{d/2} \exp \left(-\frac{m_i V^2}{2T_i} \right). \quad (10)$$

With this approximation, the integrals appearing in the expressions of the cooling rates ζ_{ij} and the collisional moments \mathbf{A}_{ij} can be explicitly evaluated. Retaining only linear terms in \mathbf{C}_i and after a lengthy calculation, one gets

$$\zeta_{ij} = \frac{2\pi^{(d-1)/2}}{d\Gamma(d/2)} n_j \mu_{ji} \sigma_{ij}^{d-1} v_0 \left(\frac{\theta_i + \theta_j}{\theta_i \theta_j} \right)^{1/2} (1 + \alpha_{ij}) \left[2 - \mu_{ji} (1 + \alpha_{ij}) \frac{\theta_i + \theta_j}{\theta_j} \right], \quad (11)$$

$$\begin{aligned} \mathbf{A}_{ij} = & -\frac{\pi^{(d-1)/2}}{d\Gamma(d/2)} m_i n_i n_j \mu_{ji} \sigma_{ij}^{d-1} v_0^3 \left(\frac{\theta_i + \theta_j}{\theta_i \theta_j} \right)^{3/2} (1 + \alpha_{ij}) \left\{ \left[\lambda_{ij} - \frac{d}{d+3} \mu_{ji} (1 + \alpha_{ij}) \right] \mathbb{1} \right. \\ & \left. + 2 \frac{\theta_i \theta_j}{(\theta_i + \theta_j)^2} \left[\left(1 + \frac{d+3}{2(d+2)} \frac{\theta_i + \theta_j}{\theta_i} \lambda_{ij} \right) \mathbf{C}_i - \left(1 - \frac{d+3}{2(d+2)} \frac{\theta_i + \theta_j}{\theta_j} \lambda_{ij} \right) \mathbf{C}_j \right] \right\}. \end{aligned} \quad (12)$$

In these expressions, $v_0 = \sqrt{2T(m_1 + m_2)/m_1 m_2}$ is a thermal velocity defined in terms of the temperature of the mixture T , and

$$\theta_1 = \frac{1 + x_1(\gamma - 1)}{\mu_{21}\gamma}, \quad \theta_2 = \frac{1 + x_1(\gamma - 1)}{\mu_{12}}, \quad (13)$$

$$\lambda_{ij} = 2 \frac{\mu_{ij}\theta_j - \mu_{ji}\theta_i}{\theta_i + \theta_j} + \frac{\mu_{ji}}{d+3} (2d+3 - 3\alpha_{ij}). \quad (14)$$

Equations (11) and (12) extend previous expressions [9] obtained in the three dimensional case. The approximation (12) allows one to solve the set of equations (8) and express \mathbf{P}_i as a function of γ , while the approximation (11) gives the cooling rates ζ_i . When all these expressions are used in Eq. (7), one gets a *closed* equation for the temperature ratio γ , that can be solved numerically.

A full presentation of the results is not possible because of the complexity of the parameter space: α_{11} , α_{22} , α_{12} , m_1/m_2 , x_1 , and σ_1/σ_2 . As in Ref. [4], we assume for the sake of illustration that the spheres or disks are made of the same material ($\alpha_{ij} = \alpha$) and have the same mass density, i.e., $m_1/m_2 = (\sigma_1/\sigma_2)^d$. This reduces the parameter space to α , x_1 , and σ_1/σ_2 . As expected, our results show that in general the kinetic temperatures of the mixture are different ($\gamma \neq 1$). There are only two trivial exceptions: the elastic case ($\alpha = 1$) and the case of mechanically equivalent particles ($m_1 = m_2$, $\sigma_1 = \sigma_2$). Beyond these cases, the dependence of γ on the parameters of the problem is quite intricate. As an illustration, we plot the temperature ratio T_1/T_2 versus the diameter ratio σ_1/σ_2 for $x_1 = \frac{1}{3}$ (Fig. 1) and $x_1 = \frac{1}{2}$ (Fig. 2) for three different values of α : $\alpha = 0.95$, $\alpha = 0.9$, and $\alpha = 0.8$. We have considered the two dimensional case ($d = 2$). Also, for comparison we show the kinetic-theory predictions of Jenkins and Mancini [6]. It is apparent that an excellent agreement between Monte Carlo simulations (symbols) and our theory is found over the entire range of values of size and mass ratios considered. Although the solid fractions considered by Clelland and Hrenya [4] prevent us from making a quantitative comparison between our theory and their simulations, we observe that the behavior of γ in dilute systems is qualitatively similar to the one found in Ref. [4]. Thus, for instance, at a given value of α the granular energy of the larger particle (say for instance, species 1) increases relative to that of the smaller particle as the size ratio σ_1/σ_2 increases. Both Monte Carlo simulation and theory show that the temperature ratio presents a strong dependence on the restitution coefficient. With respect to the influence of composition, comparison of Figs. 1 and 2 indicates that γ exhibits a very weak dependence on the mole fraction x_1 . This behavior has been also found in recent experiments [3] carried out on binary vibrated granular gases. We also see that all the above trends are qualitatively reproduced by the theory of Jenkins and Mancini [6] (which is restricted to nearly elastic disks), although these trends are however strongly exaggerated. Thus, for instance, at a size ratio $\sigma_1/\sigma_2 = 3$, in the case $x_1 = \frac{1}{2}$ and $\alpha = 0.8$, the discrepancy between our theory and the simulation is less than 1% while it is around of 115% in the theory of Jenkins and Mancini [6].

An interesting point is to assess the influence of the temperature differences on the rheological properties of the mixture. Although the comparison carried out in Ref. [4] between previous theories (based on a single temperature) and simulation shows a qualitative good agreement at the level of the shear stresses, one expects that the new contributions coming from the energy difference leads to an improvement over previous theoretical predictions. In Fig. 3, we plot the dimensionless stresses $-P_{xy}^*$ and P_{yy}^* versus the restitution coefficient in the case $x_1 = \frac{1}{2}$ and $m_1/m_2 = (\sigma_1/\sigma_2)^{1/2} = 10$. Here, $P^* = P/nT = (P_1 + P_2)/nT$. Also shown in this Fig. 3 is the result which would be obtained if the differences in the partial temperatures were neglected [i.e., $\theta_i = \mu_{ji}^{-1}$ in Eqs. (11) and (12)]. In general, inclusion of the two-temperature effects represents a significant improvement of the theory, especially in the case of the shear stress P_{xy}^* , which is the most relevant rheological property in a sheared flow problem. This justifies the use of a two-temperature description to capture the dependence of stresses on dissipation.

In summary, we have obtained an approximate evaluation of the temperature ratio of a sheared granular mixture. The accuracy of this calculation has been also confirmed by Monte Carlo simulation of the Boltzmann equation. As was also found in recent MD simulations [4], our results show that the temperature ratio strongly depends on dissipation and the

mechanical parameters of the mixture (especially on the ratios of mass and size). In addition, the effect of temperature differences on rheology is important (especially in the case of the shear stress) and leads to an improvement of the theoretical results with respect to the predictions made from a single-temperature theory.

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FIGURES

FIG. 1. Plot of the temperature ratio T_1/T_2 as a function of the size ratio $\sigma_1/\sigma_2 = (m_1/m_2)^{1/2}$ for a two-dimensional system in the case $x_1 = 1/3$ and three different values of the restitution coefficient α : (a) $\alpha = 0.95$, (b) $\alpha = 0.9$, and (c) $\alpha = 0.8$. The solid lines are the theoretical predictions while the symbols refer to the Monte Carlo simulation results. The dashed line corresponds to the prediction given by the theory of Jenkins and Mancini [6] in the case $\alpha = 0.8$.

FIG. 2. The same as in Fig. 1 but for $x_1 = 1/2$.

FIG. 3. Plot of the reduced elements of the pressure tensor $P_{yy}^* = P_{yy}/nT$ and $P_{xy}^* = P_{xy}/nT$ as a function of the restitution coefficient α for a two-dimensional system in the case $m_1/m_2 = 10$ and $x_1 = 1/2$. The solid lines are the theoretical predictions while the symbols refer to the Monte Carlo simulation results. The dashed lines correspond to the theoretical results by assuming the equality of the partial temperatures $T_1/T_2 = 1$.





